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CFDRC

PARTICULATE CONTAMINANT FORMATION AND TRANSPORT IN MICROELECTRONIC MANUFACTURING PROCESSES

Phase II Quarterly Report

by

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and

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University of Minnesota

and

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University of Illinois

September-November 1997

CFDRC Report: 4396/7

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1. INTRODUCTION

This is the seventh quarterly report documenting the work performed during a two year Phase II STTR activity entitled "Particulate contaminant formation and transport in microelectronic manufacturing processes." The overall objective is to produce a charging, transport, and growth simulation (CTGS) tool that can be used effectively by equipment manufacturers and users to reduce particle generation in fabrication systems. The project includes collaborations with Prof. Steven Girshick (University of Minnesota) on ion induced nucleation and Prof. Mark J. Kushner (University of Illinois) on particle charging and transport.

1.1 Project Objectives

The work to be performed in this Phase II STTR includes:

1. to obtain and adapt models for particle charging, particle growth, and electrostatic and ionic drag forces on particles from Prof. Mark J. Kushner's group at the University of Illinois Urbana-Champaign (UIUC);

2. to obtain and adapt models for ion-induced nucleation from Prof. Steven Girshick's group at the University of Minnesota (UMN);

3. to implement the above models into CFDRC's reactor model, CFD-ACE, to obtain solutions for local particle formation and transport in conjunction with other macroscopic processes such as fluid flow, heat/mass transfer, plasma transport and chemistry;

4. to perform detailed parametric studies to assess the effects of various operating conditions on particle formation and transport;

5. to demonstrate the integrated model in collaboration with an equipment manufacturer to reduce/eliminate particle effects in a processing system;

6. to transfer the technology to the industry in collaboration with SEMATECH and its member companies; and

7. to prepare a final report documenting the work performed during the Phase II study.

1.2 Project Status

The moment model has undergone further development allowing input of material properties of a system to be studied. The conversion of the DTS at UIUC to 3D has been finalized and consequences of 3-D structures in ICP reactors on particle traps has been studied. At UMN particle nucleation rates during LPCVD of polysilicon from silane in the

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GEC reference cell due to clustering sequences involving chemical reactions between silicon hydride species is being studied.

1.3 Overview

Section 2 describes progress made on the particle transport model by the University of Illinois sub-contractor. Section 3 describes progress made modeling nucleation pathways for use with the moment model as reported by the University of Minnesota sub-contractor. Section 4 discusses modifications made by CFDRC to the moment model. Section 5 discusses the future plans for the CTGS tool development.

2. UNIVERSITY OF ILLINOIS PROGRESS REPORT

The following is a report written at the University of Illinois documenting work done on the particle transport algorithm described here and in earlier reports.

Final modifications of DTS-3D were completed. These modifications included refinements in algorithms to speed the calculation and reduce memory requirements. Algorithms for particle-particle Coulomb interactions were ported from DTS-2D to DTS-3D. Preliminary parameterizations of the particle-particle algorithms proved to be successful, however the large number of computational particles required to implement this option will restrict its use. For example, only 1/4 "slices" of the reactor (employing reflective boundary conditions) are typically used in order to increase the particle density (for a given number of particles). We demonstrated emptying of 3-D traps in reactive-ion-etching reactors by "over-filling" the traps.

A study on the consequences of 3-D structures in ICP reactors on particle traps was reported at the American Vacuum Society Symposium in San Jose in October 1997. Results from a new parameterization were also reported in which 3-D particle traps are produced not by "geometrical" asymmetries but rather "electrical" asymmetries. The electrical asymmetries result from transmission line effects in the antenna which produce azimuthally dependent power deposition and ion fluxes. Volumetric particle traps were produced in azimuthal sectors of the reactor which have lower power deposition.

3. UNIVERSITY OF MINNESOTA PROGRESS REPORT

The following is a report written at the University of Minnesota documenting work done on the nucleation term to be included in the moment model described here and in earlier reports.

During this period numerical calculations were conducted of gas-phase and surface chemistry, and of particle nucleation rates, during LPCVD of polysilicon from silane in the GEC reference cell. In addition comparisons were obtained of different calculations which highlighted the effect on the results of assuming different kinetic mechanisms and of using different numerical schemes.

The Sandia SPIN code was used to obtain results with two different chemical mechanisms: (1) the gas-phase and surface mechanism recommended by Ho et al. (1994), and (2) the simplified kinetic mechanism used by CFDRC. Both mechanisms were tested using SPIN. While the results were similar in most respects, some significant discrepancies were found, for example the predicted hydrogen concentration differed by about two orders of magnitude for the two different chemical mechanisms. In contrast the two different numerical schemes (either CFD's or SPIN) produced quite similar results when the same chemical mechanism was assumed.

The gas phase species concentrations calculated by SPIN, together with cluster Gibbs free energies, were then used as input to atomistic nucleation models by Girshick (1997) to predict particle formation rates in the GEC reference cell reactor. Particle formation mechanisms considered were chemical nucleation by gas-phase reaction sequences involving silicon hydride radical species. Predicted nucleation rates were obtained as a function of distance from a heated susceptor.

4. MOMENT MODEL

The moment model at CFDRC has undergone modification. The code now specifies material properties through the input file instead of "hard-wired" in the code. Material properties include items such as monomer specie, monomer mass, particle density, particle conductivity, vapor pressure, and surface tension. The altered code facilitated testing the model with other material systems. Through testing tweaks to the source term were made to allow for convergence, such as limiting source terms to non-negative values.

5. FUTURE WORK

The current status of the project is shown in Table 5-1. Future work will address both areas of the technology transfer focusing on improvements to the transport, charging, and growth models.

Table 5-1. Status of Project Tasks

Task Description	2	4	6	8	10	12	14	16	18	20	22	24
Task 1. Model Transfer from UIUC												
(i) Model Transfer	X	X	X	X	X	X						
(ii) Documentation	X	X	X	X	X	X	X	X	X	X	X	X
(iii) Consultation on Model Adaptation	X	X	X	X	X	X	X	X	X	X	X	X
Task 2. Model Transfer from UMN												
(i) Ion-Induced Nucleation Model	X	X	X	X	X	X						
(ii) Model Documentation/Transfer	X	X	X	X	X	X	X	X	X	X	X	X
(iii) Consultation on Model Adaptation/Coupling	X	X	X	X	X	X	X	X	X	X	X	X
Task 3. Physical Model Development and Adaptation at CFDRC												
(i) Model for Particle Formation				X	X							
(ii) Model for Particle Transport				X	X	X						
(iii) Adaptation of UIUC and UMN Models	X	X	X	X	X	X	X					
Task 4. Coupling with CFD Code												
(i) Incorporation of Models into CFD Code	X	X	X	X	X	X	X					
(ii) Testing and Assessment of Coupled Model				X	X	X	X	X	X			
(iii) Preliminary Validation Studies							X	X	X			
(iv) Parametric Studies							X	X	X	X	X	X
Task 5. Packaging and Documentation of Coupled Model												
(i) Implementation of Graphical User Interface (GUI)										X	X	X
(ii) Detailed Documentaition of Models and Code Structure											X	X
(iii) Preparation of Final Report												X

The moment model will incorporate the atomistic nucleation model as a source term. The possibility of forming a discrete-modal model will be explored. A discrete-modal model solves separate General Dynamic Equations (GDEs) for small clusters and the moments of the GDE assuming a lognormal size distribution for particles above a specified size. Coupling a discrete model with a moment model will be explored as an option.

The GUI for the charging and transport will undergo further testing. More efficient information sharing from ACE and PLASMA(ICP) code to the transport code will be explored such as through the restart files. The transport model which currently assumes monodisperse systems will be altered to transport more than one particle size at the same time. Other modifications which have yet to be finalized could include transport of non-spherical particles (i.e., flakes), accounting for particle coulomb-coulomb interactions,

making particle charging time-dependent, changing the charging model for smaller size particles, and allow for variance in size as particles collide with each other increasing in size or atoms evaporate off of the particle reducing its size.

REFERENCES

Girshick, S. L., "Theory of nucleation from the gas phase by a sequence of reversible chemical reactions," J. Chem. Phys. 107, 1948-1952 (1997).

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CFD RESEARCH CORPORATION
Ref: ARPA Contract # MDA972-96-C-0003; CFDRC Project # 4396

Actuals

MONTHS

	1	2	3	4	5	6	7	8	9	10	11	12
	Feb-96	Mar-96	Apr-96	May-96	Jun-96	Jul-96	Aug-96	Sep-96	Oct-96	Nov-96	Dec-96	Jan-97
Labor Hours												
Current month	204	226	430	191	187	281	190	173	209	173	135	187
Contract to date	204	430	860	1051	1238	1519	1709	1882	2091	2264	2399	2586
Total Costs												
(In thousands)												
Current month	17.7	16.7	17.7	13.6	11.9	20.6	12.6	15.0	21.9	23.6	10.8	14.4
Contract to date	17.7	34.3	52.0	65.6	77.5	98.1	110.7	125.8	147.6	171.3	182.0	196.4

	13	14	15	16	17	18	19	20	21	22	23	24
	Feb-97	Mar-97	Apr-97	May-97	Jun-97	Jul-97	Aug-97	Sep-97	Oct-97	Nov-97	Dec-97	Jan-98
Labor Hours												
Current month	161	112	3	0	0	0	0	0	0			
Contract to date	2747	2859	2862	2862	2862	2862	2862	2862	2862	2862	2862	2862
Total Costs												
(In thousands)												
Current month	24.0	16.0	10.8	3.8	2.0	0.0	11.6	9.0	0.0			
Contract to date	220.4	236.4	247.2	251.0	253.0	253.0	264.6	274.0	274.0	274.0	274.0	274.0

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